**SUPPLEMENTARY MATERIAL for**

**Experimental Investigation and Modeling of Thermophysical and Extraction Properties of Choline Chloride + dl-Malic acid Based Deep Eutectic Solvent**

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**Table SI** – Experimental densities, viscosities and refractive indices for binary mixture DES (1) + methanol (2) over the temperature range between 298.15 K and 323.15 K and at atmospheric pressurea,b

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| *x*1 | *ρ /* 103 kg·m-3 | *η /* mPa∙s | *nD* | *x*1 | *ρ /* 103 kg·m-3 | *η /* mPa∙s | *nD* |
| *T=*298.15 K | | | | | | | |
| 0 | 0.787068 | 0.55577 |  | 0.6005 | 1.207312 | 775.01 | 1.46761 |
| 0.0996 | 0.922937 | 1.9947 | 1.37308 | 0.7001 | 1.225883 | 1585.5 | 1.47543 |
| 0.1999 | 1.018942 | 6.8703 | 1.40535 | 0.7990 | 1.241360 | 4682.3 | 1.48272 |
| 0.3001 | 1.094695 | 22.644 | 1.42847 | 0.8954 | 1.256641 | 11213 | 1.48808 |
| 0.3996 | 1.150458 | 96.521 | 1.44760 | 1 | 1.275061 | 22091 | 1.49378 |
| 0.4953 | 1.182521 | 246.24 | 1.45849 |  |  |  |  |
| *T=*303.15 K | | | | | | | |
| 0 | 0.782343 | 0.52224 |  | 0.6005 | 1.203896 | 538.74 | 1.46632 |
| 0.0996 | 0.918439 | 1.8046 | 1.37152 | 0.7001 | 1.222609 | 1076.8 | 1.47414 |
| 0.1999 | 1.015164 | 5.998 | 1.40372 | 0.7990 | 1.238216 | 3027.7 | 1.48146 |
| 0.3001 | 1.090789 | 18.713 | 1.42697 | 0.8954 | 1.253599 | 6825.2 | 1.48684 |
| 0.3996 | 1.147090 | 74.434 | 1.44629 | 1 | 1.272033 | 13393 | 1.49256 |
| 0.4953 | 1.179176 | 181.13 | 1.45711 |  |  |  |  |
| *T=*308.15 K | | | | | | | |
| 0 | 0.777601 | 0.48385 |  | 0.6005 | 1.200955 | 383.72 | 1.46504 |
| 0.0996 | 0.913966 | 1.6389 | 1.36978 | 0.7001 | 1.219912 | 752.6 | 1.47287 |
| 0.1999 | 1.011388 | 5.2275 | 1.40208 | 0.7990 | 1.235763 | 2012.4 | 1.48021 |
| 0.3001 | 1.087060 | 15.653 | 1.42548 | 0.8954 | 1.251382 | 4378.4 | 1.48560 |
| 0.3996 | 1.143721 | 58.429 | 1.44502 | 1 | 1.269028 | 8995 | 1.49134 |
| 0.4953 | 1.175968 | 135.98 | 1.45573 |  |  |  |  |
| *T=*313.15 K | | | | | | | |
| 0 | 0.772836 | 0.44514 |  | 0.6005 | 1.198299 | 279.56 | 1.46379 |
| 0.0996 | 0.910175 | 1.5016 | 1.36791 | 0.7001 | 1.217459 | 536.62 | 1.47160 |
| 0.1999 | 1.007611 | 4.573 | 1.40043 | 0.7990 | 1.233491 | 1372.1 | 1.47896 |
| 0.3001 | 1.083723 | 13.147 | 1.42402 | 0.8954 | 1.249263 | 2909.6 | 1.48438 |
| 0.3996 | 1.140361 | 46.505 | 1.44375 | 1 | 1.266047 | 5858.8 | 1.49012 |
| 0.4953 | 1.172761 | 104.1 | 1.45429 |  |  |  |  |
| *T=*318.15 K | | | | | | | |
| 0 | 0.768039 | 0.41030 |  | 0.6005 | 1.194398 | 208.12 | 1.46253 |
| 0.0996 | 0.905188 | 1.3649 | 1.36621 | 0.7001 | 1.213636 | 390.96 | 1.47036 |
| 0.1999 | 1.003255 | 4.1027 | 1.39885 | 0.7990 | 1.229662 | 960.47 | 1.47772 |
| 0.3001 | 1.079164 | 11.318 | 1.42251 | 0.8954 | 1.245364 | 1973.8 | 1.48317 |
| 0.3996 | 1.137015 | 37.714 | 1.44245 | 1 | 1.263089 | 4120.7 | 1.48892 |
| 0.4953 | 1.169545 | 81.18 | 1.45288 |  |  |  |  |
| *T=*323.15 K | | | | | | | |
| 0 | 0.763201 | 0.37457 |  | 0.6005 | 1.191126 | 158.78 | 1.46127 |
| 0.0996 | 0.899933 | 1.2724 | 1.36603 | 0.7001 | 1.210487 | 290.48 | 1.46921 |
| 0.1999 | 0.997821 | 3.6997 | 1.39691 | 0.7990 | 1.226518 | 690.72 | 1.47649 |
| 0.3001 | 1.074627 | 9.7934 | 1.42087 | 0.8954 | 1.242213 | 1381.4 | 1.48197 |
| 0.3996 | 1.133692 | 31.069 | 1.44120 | 1 | 1.260153 | 2923.8 | 1.48764 |
| 0.4953 | 1.166317 | 64.745 | 1.45159 |  |  |  |  |

a Standard uncertainties *u* for each variable are: *u*(*T*) = 0.01 K; *u*(*p*) = 5 %; *u*(*x1*) = 0.0001, and the combined expanded uncertainties *Uc* are *Uc*(*ρ*) = 4×10-2 kg⋅m-3; *Uc*(*nD*) = 9×10-5 and *Uc*(*η*) = 1.0 %, with 0.95 level of confidence (k ≈ 2); b Empty cells indicate values out of the measuring range of the apparatus.

**Table SII** – Experimental densities, viscosities and refractive indices for binary mixture water (1) + DES (2) over the temperature range between 298.15 K and 363.15 K and at atmospheric pressurea,b

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| *x*1 | *ρ /* 103 kg·m-3 | | *η /* mPa∙s | *nD* | *ρ /* 103 kg·m-3 | *η /* mPa∙s | | *nD* | *ρ /* 103 kg·m-3 | *η /* mPa∙s | | *nD* | |
| *T=*298.15 | | | | | *T=*303.15 | | | | *T=*308.15 | | | |
| 0 | | 1.275061 | 22091 |  | 1.272033 | 13393 |  | | 1.269028 | 8995 |  | | |
| 0.1930 | | 1.267518 | 8100.0 | 1.48865 | 1.264472 | 5343.7 | 1.48742 | | 1.261449 | 3454.4 | 1.48620 | | |
| 0.2956 | | 1.260061 | 3713.0 | 1.48440 | 1.256997 | 2261.8 | 1.48317 | | 1.253954 | 1510.5 | 1.48195 | | |
| 0.3983 | | 1.252732 | 1247.7 | 1.47943 | 1.249662 | 848.10 | 1.47820 | | 1.246609 | 591.76 | 1.47697 | | |
| 0.4585 | | 1.247395 | 695.01 | 1.47604 | 1.244312 | 486.27 | 1.47480 | | 1.241233 | 349.13 | 1.47359 | | |
| 0.5142 | | 1.240114 | 397.76 | 1.47156 | 1.236999 | 286.67 | 1.47034 | | 1.233883 | 210.99 | 1.46913 | | |
| 0.5751 | | 1.231732 | 233.95 | 1.46711 | 1.228575 | 185.03 | 1.46587 | | 1.225548 | 154.05 | 1.46463 | | |
| *T=*313.15 | | | | | *T=*318.15 | | | | *T=*323.15 | | | |
| 0 | | 1.266047 | 5858.8 |  | 1.263089 | 4120.7 |  | | 1.260153 | 2923.8 |  | | |
| 0.1930 | | 1.258448 | 2293.9 | 1.48499 | 1.255468 | 1565.4 | 1.48378 | | 1.252506 | 1094.9 | 1.48258 | | |
| 0.2956 | | 1.250925 | 1035.4 | 1.48073 | 1.247912 | 727.96 | 1.47951 | | 1.244905 | 523.54 | 1.47830 | | |
| 0.3983 | | 1.243561 | 423.15 | 1.47576 | 1.240514 | 309.51 | 1.47453 | | 1.237467 | 230.93 | 1.47333 | | |
| 0.4585 | | 1.238154 | 256.59 | 1.47236 | 1.235072 | 191.98 | 1.47116 | | 1.232108 | 146.47 | 1.46995 | | |
| 0.5142 | | 1.230874 | 159.20 | 1.46790 | 1.227897 | 122.92 | 1.46670 | | 1.224906 | 96.029 | 1.46549 | | |
| 0.5751 | | 1.222542 | 115.04 | 1.46339 | 1.219511 | 87.671 | 1.46214 | | 1.21647 | 68.028 | 1.46089 | | |
| *T=*328.15 | | | | | *T=*333.15 | | | | *T=*338.15 | | | |
| 0 | | 1.257025 | 2024.4 |  | 1.254030 | 1486.1 |  | | 1.251035 | 1070.9 |  | | |
| 0.1930 | | 1.249562 | 782.49 | 1.48139 | 1.246632 | 571.46 | 1.48022 | | 1.243709 | 425.43 | 1.47906 | | |
| 0.2956 | | 1.241906 | 384.62 | 1.47709 | 1.23891 | 288.37 | 1.47591 | | 1.235908 | 220.12 | 1.47472 | | |
| 0.3983 | | 1.234435 | 175.52 | 1.47211 | 1.231526 | 135.65 | 1.47094 | | 1.228609 | 106.55 | 1.46977 | | |
| 0.4585 | | 1.229171 | 113.66 | 1.46877 | 1.226218 | 89.807 | 1.46756 | | 1.223258 | 71.800 | 1.46639 | | |
| 0.5142 | | 1.221912 | 76.184 | 1.46428 | 1.21892 | 61.294 | 1.46307 | | 1.215921 | 50.154 | 1.46187 | | |
| 0.5751 | | 1.213409 | 53.875 | 1.45966 | 1.210316 | 43.390 | 1.45845 | | 1.207159 | 35.474 | 1.45725 | | |
| *T=*343.15 | | | | | *T=*348.15 | | | | *T=*353.15 | | | |
| 0 | | 1.248040 | 813.29 |  | 1.245045 | 613.83 |  | | 1.242050 | 482.51 |  | | |
| 0.1930 | | 1.240790 | 321.82 | 1.47793 | 1.237871 | 247.37 |  | | 1.234950 | 193.02 |  | | |
| 0.2956 | | 1.232907 | 170.54 | 1.47361 | 1.229908 | 134.081 |  | | 1.226909 | 106.84 |  | | |
| 0.3983 | | 1.225680 | 84.797 | 1.46892 | 1.222756 | 68.382 |  | | 1.219824 | 55.778 |  | | |
| 0.4585 | | 1.220300 | 58.108 | 1.46530 | 1.217341 | 47.570 |  | | 1.214383 | 39.214 |  | | |
| 0.5142 | | 1.212911 | 41.156 | 1.46071 | 1.209891 | 34.263 |  | | 1.206861 | 28.774 |  | | |
| 0.5751 | | 1.203804 | 29.320 | 1.45610 | 1.200556 | 24.490 |  | | 1.197423 | 20.652 |  | | |
| *T=*358.15 | | | | | *T=*363.15 | | | |  | | | |
| 0 | | 1.239055 | 375.58 |  | 1.236060 | 300.95 |  | |  |  |  | | |
| 0.1930 | | 1.232047 | 152.78 |  | 1.229219 | 123.34 |  | |  |  |  | | |
| 0.2956 | | 1.223903 | 86.213 |  | 1.220891 | 70.321 |  | |  |  |  | | |
| 0.3983 | | 1.216887 | 46.015 |  | 1.213944 | 38.628 |  | |  |  |  | | |
| 0.4585 | | 1.211409 | 32.522 |  | 1.208444 | 27.120 |  | |  |  |  | | |
| 0.5142 | | 1.203826 | 24.234 |  | 1.200823 | 19.286 |  | |  |  |  | | |
| 0.5751 | | 1.194302 | 17.547 |  | 1.191271 | 14.635 |  | |  |  |  | | |

a Standard uncertainties *u* for each variable are: *u*(*T*) = 0.01 K; *u*(*p*) = 5 %; *u*(*x1*) = 0.0001, and the combined expanded uncertainties *Uc* are *Uc*(*ρ*) = 4×10-2 kg⋅m-3; *Uc*(*nD*) = 9×10-5 and *Uc*(*η*) = 1.0 %, with 0.95 level of confidence (k ≈ 2); b Empty cells indicate values out of the measuring range of the apparatus.

**Table SIII** – Experimental viscosities for the mixture DES + glycerol (choline chloride:dl-malic acid:glycerol in molar ratio 1:1:0.5) over the temperature range between 298.15 K and 363.15 K and at atmospheric pressurea

|  |  |
| --- | --- |
| T / K | *η /* mPa∙ s |
| 298.15 | 10271 |
| 303.15 | 6351.6 |
| 308.15 | 4032.7 |
| 313.15 | 2668.2 |
| 318.15 | 1801.7 |
| 323.15 | 1247.7 |
| 328.15 | 884.36 |
| 333.15 | 640.31 |
| 338.15 | 472.54 |
| 343.15 | 355.17 |
| 348.15 | 271.39 |
| 353.15 | 210.66 |
| 358.15 | 165.85 |
| 363.15 | 133.12 |

a Standard uncertainties *u* for each variable are: *u*(*T*) = 0.01 K; *u*(*p*) = 5 %; and the combined expanded uncertainty *Uc Uc*(*η*) = 1.0 %, with 0.95 level of confidence (k ≈ 2).

**Table SIV** – Parameters of viscosity fitting using Vogel-Fulcher-Tammann model, goodness of fit statistic *R*2 and energy of activation of viscous flow *Ea,η* for the system DES+Glycerol (choline chloride:dl-malic acid:glycerol is in molar ratio 1:1:0.5)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | *A* | *B* | *T*0 / K | *R*2 |
|  | -3.5330 | 1612.0000 | 172.0000 | 0.9998 |
| *T* / K | *Ea,η* / kJ·mol-1 | | | |
| 298.15 | 74.87 | 338.15 | 55.52 |  |
| 303.15 | 71.61 | 343.15 | 53.88 |  |
| 308.15 | 68.66 | 348.15 | 52.36 |  |
| 313.15 | 65.97 | 353.15 | 50.94 |  |
| 318.15 | 63.51 | 358.15 | 49.61 |  |
| 323.15 | 61.26 | 363.15 | 48.38 |  |
| 328.15 | 59.19 |  |  |  |

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